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A Computer Program
for Analyzing Unresolved
Mössbauer Hyperfine Spectra

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for Analyzing Unresolved
Mössbauer Hyperfine Spectra**

**James R. Schiess and Jag J. Singh
Langley Research Center
Hampton, Virginia**



**National Aeronautics
and Space Administration**

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SUMMARY

A computer program has been developed for analyzing unresolved Mössbauer hyperfine spectra resulting from the existence of several local environments in dilute binary iron alloys. This program is an extension of an earlier program which had not been adapted for analyzing such unresolved compound spectra. The program is written in FORTRAN IV language for the Control Data CYBER 170 series digital computer system with network operating system (NOS) 1.1. With the present dimensions, the program requires approximately 36000 octal locations of core storage. A typical case involving two innermost coordination shells in which the amplitudes and the peak positions of all three components are estimated in 25 iterations requires 30 seconds on CYBER 173. The program has been applied to determine the effects of various near-neighbor impurity shells on hyperfine fields in dilute FeAl alloys.

INTRODUCTION

The effects of impurity atoms on iron Mössbauer spectra have been under investigation at the Langley Research Center for quite some time. (See refs. 1 to 5.) In these studies, various types of impurity atoms in dilute concentrations (less than 6 atomic percent) were introduced into the absorber iron lattice and the Mössbauer spectra recorded. From such spectra, the effective values of three critical Mössbauer parameters - hyperfine field, isomer shift, and outer peak widths - were determined. These measurements have shown that (1) the effective hyperfine field and the isomer shift in iron decrease as the concentration of nonmagnetic impurity atoms increases and (2) the effective peak width shows linear increase with increasing impurity concentration. The effective values of Mössbauer parameters were obtained by analyzing the experimental spectrum as a single six-peak Mössbauer spectrum, even though it was a composite spectrum resulting from the superimposition of spectra from several iron-with-near-neighbor configurations. The analysis was performed using the program D3290 described in an earlier report (ref. 6). Such an approach necessarily combines the effects of near-neighbor impurity atoms at various sites in the iron lattice.

It would be preferable to resolve the composite iron alloy spectrum into single-configuration spectra so that the effects of impurity atoms in various configurations could be separated. Such an analysis would allow a determination of the most important impurity sites that affect critical Mössbauer parameters. It would also permit an elucidation of the mechanisms responsible for affecting the Mössbauer parameters. For example, it may be possible to explain why impurity atoms at different distances sometimes have opposite effects on hyperfine fields at the iron nuclei. The existing program (D3290) could not analyze an unresolved hyperfine spectrum into its constituents. A computer program that can separate individual unresolved composite peaks into constituent Lorentzians has now been developed and applied to the study of FeAl alloys.

This report describes the program (MOSS2) and provides information necessary to use it.

SYMBOLS

A	amplitude of absorption peak
a	coefficient of second-order term in equation of parabola
b	coefficient of first-order term in equation of parabola
c	constant term in equation of parabola
C	impurity atomic fraction
C_j	$= (\lambda_j)^2$
H	magnetic field at absorber nucleus
H_{eff}	effective magnetic field at absorber nucleus
H_{Fe}	magnetic field at absorber nucleus in pure iron
H_i	magnetic field at absorber nucleus in iron alloy corresponding to ith impurity-atom configuration
K	a constant signifying effect of impurity atoms in coordination shells beyond 3rd near-neighbor shell
L	Lorentzian profile
l	number of impurity atoms in 1st near-neighbor shell
m	number of impurity atoms in 2nd near-neighbor shell
s	number of impurity atoms in 3rd near-neighbor shell
N	number of absorption peaks in experimental spectrum
N_{max}	maximum number of atoms in a near-neighbor shell
n	number of total atomic configurations involved in the spectrum
P	position of peak on x-axis
P_i	probability for ith impurity-atom configuration
$p(q)$	probability for q impurity atoms in near-neighbor shell
x	independent variable, source velocity

y dependent variable, counts/velocity interval
 α hyperfine field coefficient for 1st near-neighbor impurity atom
 β hyperfine field coefficient for 2nd near-neighbor impurity atom
 γ hyperfine field coefficient for 3rd near-neighbor impurity atom
 Γ width of peak at half maximum amplitude
 ϵ measurement error in L
 λ_j half of peak width at half maximum amplitude for j th peak
 Subscript:
 o nominal conditions
 Superscript:
 T transpose of matrix
 Abbreviation:
 nn near neighbor

PROBLEM DESCRIPTION

From reference 6, a single hyperfine Mössbauer spectrum can be expressed as follows:

$$y(x) = (ax^2 + bx + c) + \sum_{j=1}^N \frac{A_j}{1 + \left(\frac{P_j - x}{\lambda_j}\right)^2} \quad (1)$$

where N is the number of absorption peaks in the spectrum. When the spectrum consists of a multiple set of unresolved sextets, equation (1) must be modified as follows:

$$y(x) = (ax^2 + bx + c) + \sum_{j=1}^6 \left[\sum_{i=0}^{n-1} \frac{A_{ji}}{1 + \left(\frac{P_{ji} - x}{\lambda_j}\right)^2} \right] \quad (2)$$

In this equation, each of the six hyperfine peaks is made up of n Lorentzians defined as follows:

$$L_j \equiv \frac{A_j}{1 + \left(\frac{P_j - x}{\lambda_j}\right)^2} = \sum_{i=0}^{n-1} p_i \frac{A_j}{1 + \left(\frac{P_{ji} - x}{\lambda_j}\right)^2} = \sum_{i=0}^{n-1} c_j \frac{p_i A_j}{c_j + (P_{ji} - x)^2}$$

$$= \sum_{i=0}^{n-1} c_j \frac{A_{ji}}{c_j + (P_{ji} - x)^2} \quad (3)$$

where

- A_{ji} amplitude of i th component of j th peak of hyperfine spectrum, $p_i A_j$
- A_j amplitude of j th peak for single sextet spectrum (i.e., when iron has no near-neighbor impurity atoms)
- C_j $(\lambda_j)^2 = (\Gamma/2)^2$
- P_{ji} position on x -axis of i th component of j th peak
- P_j position on x -axis of j th peak of single sextet spectrum
- P_i probability for i th impurity-atom configuration
- λ_j half of peak width at half maximum amplitude for j th peak

In equations (2) and (3), n designates the total number of distinct atomic configurations affecting the Mössbauer spectrum of absorber iron atoms.

The analysis problem can be simplified greatly if the parabola term is eliminated from equation (2). This can be done by estimating the parabola coefficients with program D3290 (ref. 6). When the estimated parabola is subtracted from the observed spectrum, the remainder consists of six unresolved composite Lorentzians. Generally, the two outermost peaks are the best resolved lines in the spectrum and lend themselves to easy analysis. For the purpose of resolving these composite peaks, initial estimates of A_{ji} , P_{ji} , and C_j are needed. These initial estimates are obtained as follows:

(1) Initial estimate of A_{ji} :

$$A_{ji} = p_i A_j \quad (4)$$

where

$$p_i = p(\ell, m, s, \dots) = p(\ell) p(m) p(s) \dots \quad (5)$$

where

$p(l)$ probability for l impurity atoms in 1 nn shell

$p(m)$ probability for m impurity atoms in 2 nn shell

$p(s)$ probability for s impurity atoms in 3 nn shell

Assuming the absorber alloy to be a random binary mixture of the two types of atoms, probability for any given number, say q , of impurity atoms in a selected coordination shell, is given by the following expression:

$$p(q) = \binom{N_{\max}}{q} C^q (1 - C)^{N_{\max} - q}$$

$$= \frac{N_{\max}!}{q! (N_{\max} - q)!} C^q (1 - C)^{N_{\max} - q} \quad (6)$$

where N_{\max} is maximum allowed atomic population in a near-neighbor shell and C is the impurity atomic fraction. Thus for any impurity-atom configuration, p_i can be calculated from equations (5) and (6). An initial estimate of A_j is obtained from the experimental spectrum by analyzing it as a single six-peak spectrum with computer program D3290 (ref. 6).

(2) Initial estimate of P_{ji} :

$$P_{ji} = P_j \frac{H_i}{H_{Fe}} \quad (7)$$

It is shown in reference 3 that H_i , the hyperfine field corresponding to the i th impurity-atom configuration, is

$$H_i = H_{Fe} [(1 + \alpha l + \beta m + \gamma s)(1 + KC)] \quad (8)$$

where H_{Fe} represents the pure iron field obtained from the pure iron spectrum using program D3290 (ref. 6), l , m , and s represent impurity-atom populations of 1 nn, 2 nn, and 3 nn shells, α , β , and γ represent corresponding field effect coefficients, K is a constant that signifies the effect of all remaining coordination shells, and C is the impurity atomic fraction. But equation (8) cannot be used to obtain estimates of H_i in the absence of information about α , β , γ , and K . However, it has been shown in reference 3 that the effective magnetic field H_{eff} is given by

$$H_{eff} = \frac{\sum_{i=0}^{n-1} P_i H_i}{\sum_{i=0}^{n-1} P_i} \quad (9)$$

Initial estimates of H_{eff} are obtained from the experimental spectrum using program D3290. By combining this information with the calculated values of p_i , initial estimates of H_i are made. In equation (7), H_{eff} may be used as the initial estimate for H_{Fe} ; of course, H_{Fe} can be obtained from the spectrum for pure iron. An initial estimate of P_j is obtained from the experimental spectrum by analyzing it as a single six-peak spectrum with program D3290. Combining the values of H_{eff} , H_i , and P_j yields an initial estimate of P_{ji} .

(3) Initial estimate of C_j : An initial estimate of C_j is obtained from the pure iron spectrum using the program D3290 (ref. 6). It is assumed that C_j is independent of the impurity-atom configuration in the absorber lattice.

The hyperfine field for iron alloys containing significant impurity atoms (i.e., greater than 5 atomic percent) is given by equation (8). However, when the impurity concentration is low (less than 2 atomic percent), this equation can be modified as follows:

$$H_i = H_{Fe} [(1 + \alpha l + \beta m)(1 + KC)] \quad (10)$$

This equation implies that at low impurity concentrations, only impurity populations in the 1 nn and 2 nn shells have significant effect on the Mössbauer spectrum of the alloy. Specifically, one need consider only the following impurity-atom configurations: (0,0), (0,1), and (1,0). Each experimental peak can then be assumed to be made of three peaks whose intensities are determined by the probabilities for the corresponding impurity-atom configurations. Thus, for the purpose of analyzing unresolved spectra of low-impurity-concentration alloys, equation (3) can be simplified as follows:

$$L_j = \sum_{i=0}^2 C_j \frac{A_{ji}}{C_j + (P_{ji} - x)^2} \quad (11)$$

The two outer peaks (peaks 1 and 6) of the composite experimental spectrum are then least-squares-fitted to the sum of three Lorentzian peaks whose relative amplitudes are reasonably close to the estimated values of A_{ji} and whose positions are consistent with the initial estimates of P_{ji} . As indicated previously, the three Lorentzians are assumed to have the same width C_j - a justifiable assumption since the line width in Mössbauer spectra is independent of lattice spectrum in the first approximation.

Since equation (11) is nonlinear in several of the parameters, a nonlinear method was required to estimate the optimal value of the three parameters. For this reason the least-squares differential correction method was applied to this problem. A detailed description of the method is given in appendix A.

PROGRAM DESCRIPTION

The computer program MOSS2 is written in FORTRAN IV language for the Control Data CYBER 170 series digital computer system with network operating system

(NOS) 1.1. With the present dimensions, the program requires approximately 36000 octal locations of core storage. A typical case in which the amplitudes and peak positions of all three components are estimated in 25 iterations requires 30 seconds on CYBER 173.

By using initial estimates for the parameters as input to the program, a solution is obtained. The amplitude, the position of the peak on the x-axis, and the square of the width of the peak at half maximum amplitude are the parameters which may optionally be determined. The program allows a maximum of three component peaks (nine parameters) and 201 measured dependent and independent values. DIMENSION statements are easily changed to incorporate more measurements. In addition, the program allows input parameters describing an adjacent peak and a base parabola, so that these effects may be subtracted from the measured dependent values. These are obtained from program D3290 described in reference 6.

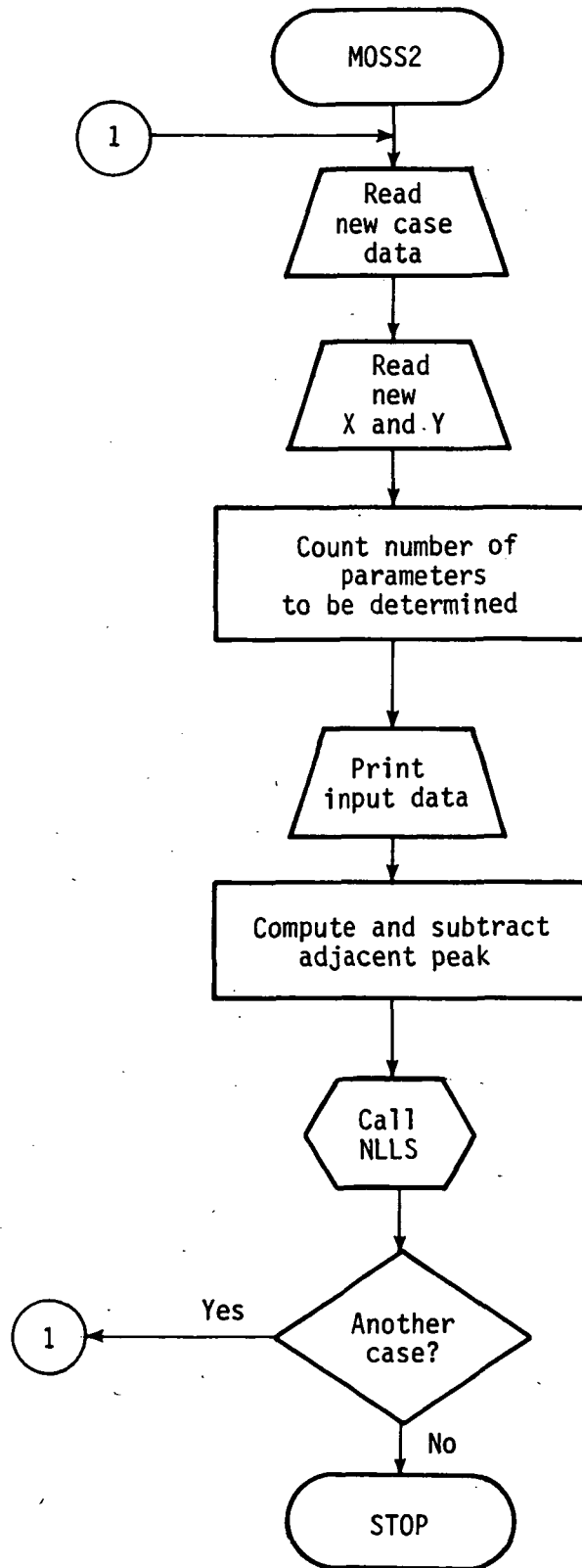
Description of FORTRAN Variables

The following list contains a description of the significant FORTRAN variables appearing in the program. The dimensions for each array are beside the variable in parentheses. The variables which are input will not be presented here, since they are described in a subsequent section.

<u>FORTRAN variable</u>	<u>Description</u>
A(201,9)	Matrix of partial derivatives
C(9,9)	Matrix of coefficients for solution of simultaneous equations
DP(9)	Right side solution of simultaneous equations
DY(201)	Residuals
SUM	Sum of squares of residuals
TP(9)	Parameter values before correction by most recent least-squares iteration
YP(201)	Dependent values computed from mathematical model

Flow Charts and Listings of Program

Program MOSS2.-- MOSS2 is the main program. It reads and prints the input, prepares for the least-squares iterations, and calls subroutine NLLS. Upon return from NLLS, the program determines whether further cases are to be attempted. The flow chart and listing of MOSS2 follow.



```

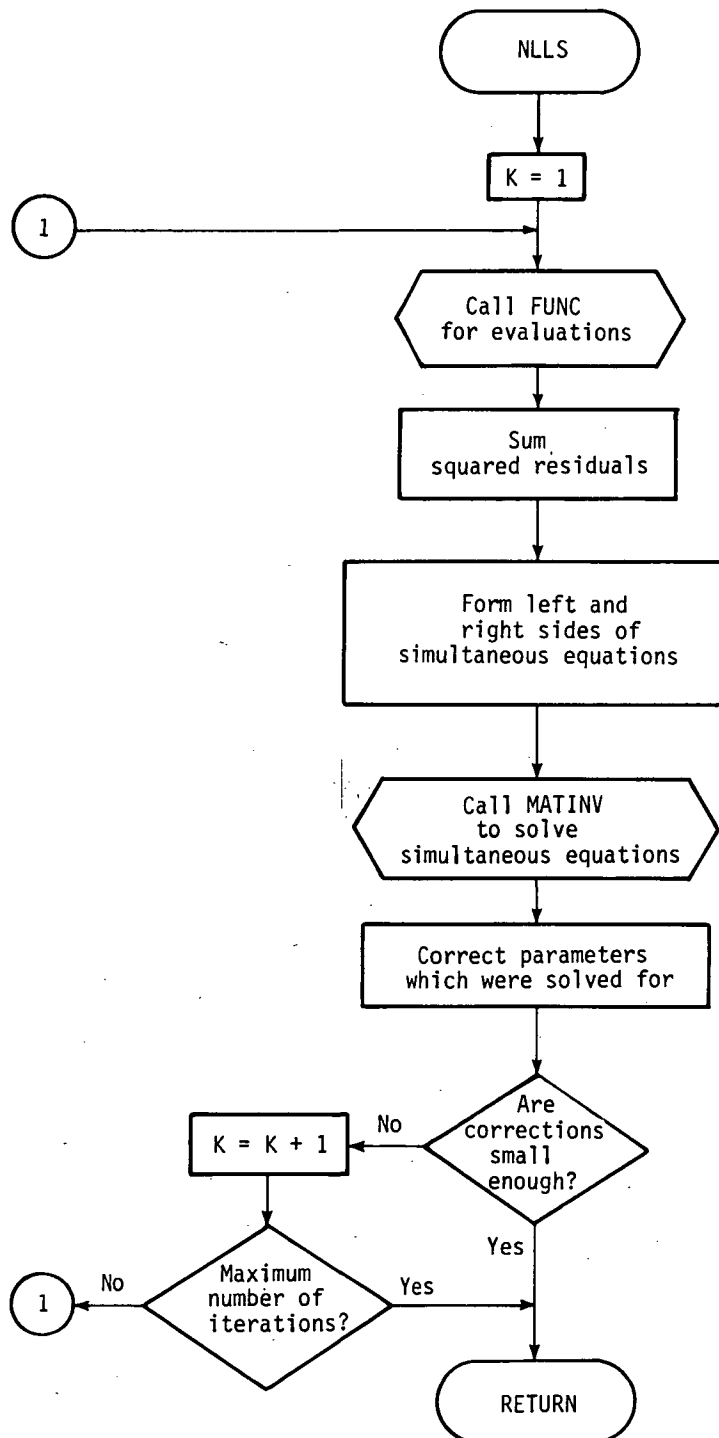
1      PROGRAM MOSS2 (INPUT,OUTPUT,TAPE5=INPUT,TAPE6=OUTPUT)
      COMMON A(201,9), DY(201), DP(9), N, M, P(12), DELTAP(9), TP(9),
1      IPAR(9), IT, EPS, X(201), Y(201), YP(201), PA,PB,PC
      DIMENSION TITLE(8)
5      DATA MMAX, NMAX/201,9/

      C
      DO 2 J=1,201
      X(J)=0.
      2   Y(J)=0.

10     C
      1 READ 6, (TITLE(J),J=1,8)
      6 FORMAT(8A10)
      IF(EOF(5)) 999,4
      4 CONTINUE
15     READ 10, IT,M,EPS
      10 FORMAT(2I10,E20.10)
      READ 11, IPAR
      11 FORMAT(9I5)
      DO 30 I=1,12
      20 READ 20, P(I)
      20 FORMAT(F25.14)
      30 CONTINUE
      READ 31, PA,PB,PC
      31 FORMAT(3E16.8)
25     READ 32, (X(J),Y(J),J=1,M)
      32 FORMAT(2E15.8)
      C
      COUNT NUMBER OF PARAMETERS TO FIND
      N=0
      DO 65 J=1,9
      30 IF(IPAR(J) .EQ. 1) N=N+1
      65 CONTINUE
      C
      PRINT 49, (TITLE(J),J=1,8)
      49 FORMAT(1H1//8A10//)
      PRINT 50, IT,M,N,EPS
35     50 FORMAT(6H IT =,I2,4H M=,I4,4H N=,I2,6H EPS=,E20.10)
      PRINT 51, IPAR
      51 FORMAT(+ DELETION FLAGS... 0=DELETE, 1=SOLVE+/(3I10))
      DO 60 I=1,12
      40 PRINT 55, (I,P(I))
      55 FORMAT(5H P(,I2,1H),1X,E18.10)
      60 CONTINUE
      PRINT 59, PA,PB,PC
      59 FORMAT(26H PARABOLA PARAMETERS PA=,E20.8,4H PB=,E20.8,4H PC=,E20
45     1.8)
      PRINT 61, (X(J),J=1,M)
      PRINT 62, (Y(J),J=1,M)
      61 FORMAT(1H0,2H X/(6E20.8))
      62 FORMAT(1H0,2H Y/(6E20.8))
50     C
      C
      SUBTRACT EFFECT OF ADJACENT PEAK FROM DATA
      DO 75 J=1,M
      ADJ= P(10)*P(12)/( P(12) +(X(J)-P(11))*2 )
      75 Y(J)=Y(J) -ADJ
55     C
      CALL NLLS(NMAX,MMAX)
      GO TO 1
      999 STOP
      END

```

Subroutine NLLS.— Subroutine NLLS controls the least-squares iterations by counting the number of iterations, calling for function and partial-derivative evaluations, solving the simultaneous equations, and correcting the parameters being determined. Also, this subroutine prints the results of each iteration. The flow chart and listing of NLLS follow.



```

1      SUBROUTINE NLLS(NMAX,MMAX)
      C
      C      NON-LINEAR LEAST SQUARES (ITERATED)
      C
5      COMMON A(201,9), DY(201), DP(9), N, M, P(12), DELTAP(9), TP(9),
      1 IPAR(9), IT, EPS, X(201), Y(201), YP(201), PA,PB,PC
      DIMENSION C(9,9), IPIV(9), IWK(18)
      DIMENSION ABC(9)
      DATA (ABC(J),J=1,9)/10H A0      ,10H P0      ,10H C0      ,10H
10     1A1      ,10H P1      ,10H C1      ,10H A2      ,10H P2      ,10H
      210H C2      /
      DATA IP,MMM/1,1/
      C
      DO 100 KK=1,IT
15     PRINT 11, KK
      11 FORMAT(1H1,40X,*ITERATION *14)
      CALL FUNC
      SUM=0.
      DO 31 J=1,M
20     31 SUM = SUM + DY(J)**2
      PRINT 32,SUM
      32 FORMAT(1H0,* SUM-OF-SQUARES *E20.7)
      DO 20 I=1,N
      C      FORM DP = A(TRANPOSE)*DY
25     DP(I)=0.
      DO 14 L=1,M
      14 DP(I)=DP(I) + A(L,I)*DY(L)
      C      FORM C= A(TRANPOSE)*A
      DO 19 J=1,N
30     C(I,J)=0.
      DO 19 L=1,M
      19 C(I,J)= C(I,J) + A(L,I)*A(L,J)
      20 CONTINUE
      CALL MATINV(NMAX,N,C,MMM,DP,IP,DET,ISC,IPIV,IWK)
35     IF(DET .NE. 0.) GO TO 103
      PRINT 101, DET
      101 FORMAT(5H DET=,E15.7,* STOP *)
      STOP
      103 CONTINUE
      PRINT 102, (C(J,J),J=1,N)
40     102 FORMAT(10H VARIANCES,6E16.7/3E16.7)
      DO 110 J=1,N
      SUM = SQRT( C(J,J))
      DO 110 L=1,N
45     C(J,L)= C(J,L)/SUM
      C(L,J)= C(L,J)/SUM
      110 CONTINUE
      PRINT 111
      111 FORMAT(1H ,* CORRELATIONS *)
50     DO 120 J=1,N
      PRINT 112,(C(J,L),L=1,N)
      120 CONTINUE
      112 FORMAT(1H ,9E14.7)
      C
55     C      LINE-UP CORRECTIONS
      K=1
      DO 10 J=1,9
      IF(IPAR(J)) 9,9,5
      5 DELTAP(J)=DP(K)
      K=K+1
      GO TO 10
      9 DELTAP(J)=0.
60     10 CONTINUE

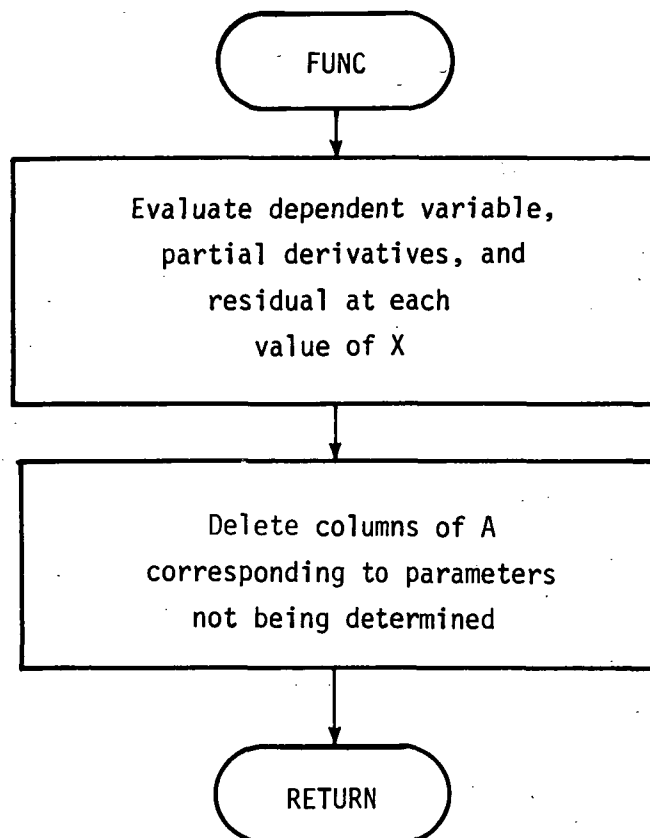
```

```

65      DO 470 I=1,9
        DP(I)=DELTAP(I)
470      P(I)=TP(I)+ DP(I)
        PRINT 520
520      FORMAT(/,1X,*ELEMENT NAME*,14X,*OLD VALUE*,21X,*INCREMENT*,
        .21X,*NEW VALUE*,/)
70      PRINT 550, (ABC(J),TP(J),DP(J),P(J),J=1,9)
550      FORMAT(1H0,(A10,8X,E21.14,9X,E21.14,9X,E21.14))
C
C      IF ALL PARAMETER CORRECTIONS LESS THAN EPS STOP
        DO 600 J=1,N
75      IF( ABS(DP(J)) .GE. EPS) GO TO 999
600      CONTINUE
        PRINT 601,EPS
601      FORMAT(27H ALL CORRECTIONS LESS THAN ,E15.7,7H STOP.)
        RETURN
80      999 CONTINUE
        100 CONTINUE
        RETURN
        END

```

Subroutine FUNC.— Subroutine FUNC uses the parameters to evaluate the predicted dependent variable and all the partial derivatives and evaluates the residuals. The matrix of partial derivatives is compressed according to which parameters are not to be determined. The flow chart and listing of FUNC follow.



```

1      SUBROUTINE FUNC
      COMMON A(201,9), DY(201), DP(9), N, M, P(12), DELTAP(9), TP(9),
1 IPAR(9), IT, EPS, X(201), Y(201), YP(201), PA,PB,PC
      C
      C      EVALUATE FUNCTION AND PARTIALS
      C
      DO 60 I=1,9
60    TP(I)=P(I)
      C
      DO 10 J=1,M
10    YP(J)=0.
      DO 7 K=1,3
      L=3*K
      L2=L-2
15    DD= P(L-1)-X(J)
      C      PARTIAL WITH RESPECT TO A(K)
      A(J,L2)= P(L)/(P(L)+DD**2)
      YP(J)= YP(J)+ P(L2)*A(J,L2)
      C      PARTIAL WITH RESPECT TO P(K)
20    A(J,L2+1)= -2.*DD*P(L2)*A(J,L2)/(P(L)+DD**2)
      C      PARTIAL WITH RESPECT TO C(K)
      A(J,L) = P(L2)*DD**2/( (P(L)+DD**2)**2 )
      7 CONTINUE
      C      ADD PARABOLA TO FUNCTION
25    YP(J)= YP(J)+ PA*X(J)**2 +PB*X(J) +PC
      C      RESIDUAL
      DY(J)= Y(J)-YP(J)
10    CONTINUE
      C
30    C      DELETE PARAMETERS
      C
      K=0
      DO 40 I=1,9
      IF( IPAR(I) ) 40,40,20
35    20 CONTINUE
      C      SAVE COLUMN I BY MOVING TO COLUMN K
      K=K+1
      DO 29 J=1,M
29    A(J,K)= A(J,I)
40    40 CONTINUE
      RETURN
      END

```

Subroutine MATINV.- Subroutine MATINV is described in detail in appendix B. Subroutine NLLS uses this subroutine to invert and solve the matrix of normal equations.

PROGRAM USAGE

Input

All the data are input to MOSS2 by using FORTRAN READ statements. For all the input variables that follow, the format used is shown in parentheses.

<u>Card</u>	<u>FORTRAN variable</u>	<u>Description</u>	<u>Format</u>
1	TITLE	Case identification	(8A10)
2	IT	Maximum number of iterations	(2I10, E20.10)
	M	Number of data-points	
	EPS	Stopping criteria; the program stops iterating on this case if the abso- lute value of each correction is less than EPS	
3	IPAR	Deletion flag: for $1 \leq I \leq 9$, IPAR(I) = 0 Do not solve for Ith parameter = 1 Solve for Ith parameter	(9I5)
4	P(1)	Amplitude of first component peak	(F25.14)
5	P(2)	Position of first component peak	(F25.14)
6	P(3)	Square of half-width of first compo- nent peak	(F25.14)
7 to 12	P(4) to P(9)	Amplitude, position, and square of half-width for second and third com- ponent peaks (same order as cards 4 to 6)	(F25.14)
13 to 15	P(10) to P(12)	Amplitude, position, and square of half-width for adjacent peak (same order as cards 4 to 6)	(F25.14)
16	PA PB PC	Coefficients of parabola, $ax^2 + bx + c$	(3E16.8)
Next M cards	X Y	Independent variable x Dependent variable y	(2E15.8)

Output

An example of the output is shown in appendix C. Explanations of output headings are as follows:

<u>Heading</u>	<u>Description</u>
Case identification	Identification given in TITLE
IT	Input value of IT

<u>Heading</u>	<u>Description</u>
M	Input value of M
N	Number of parameters to be determined
EPS	Input value of EPS
DELETION FLAGS . . .	Input values in IPAR(1) to IPAR(9)
P(1) to P(12)	Input values in P(1) to P(12)
PARABOLA PARAMETERS	
PA	Input value of PA
PB	Input value of PB
PC	Input value of PC
X	Input values of X
Y	Input values of Y

The following information is printed for each iteration:

<u>Heading</u>	<u>Description</u>
ITERATION	Iteration number
SUM-OF-SQUARES	Value of the sum of squared residuals for the current iteration
VARIANCES	Value of the parameter variances given by the least-squares procedure
CORRELATIONS	Correlation matrix for the parameters
ELEMENT NAME	Names of the individual parameters
OLD VALUE	Parameter values at the beginning of the least-squares iteration
INCREMENT	Parameter corrections obtained by least-squares iteration if parameter was to be determined; if parameter was not to be determined, a zero is printed
NEW VALUE	Parameter values after parameters are updated with correction values

If the program stops iterating because all the corrections fulfill the stopping criteria, the following message is printed:

ALL CORRECTIONS LESS THAN (Value of EPS) STOP.

The program stops and goes on to the next case if either the stopping criteria is attained or the maximum number of iterations have been attempted.

Applications

Mössbauer spectra of FeAl alloys containing 0.5, 1.0, 1.5, and 2.0 atomic percent aluminum were studied with a conventional constant-acceleration transmission Mössbauer spectrometer. The two outer peaks were analyzed into three constituent Lorentzians at each impurity concentration. From the positions of the three Lorentzian peaks, the hyperfine field values in iron resulting from 1 nn and 2 nn aluminum atoms were determined. The results are summarized in tables I and II and are shown for the 2.0-percent aluminum alloy in figures 1 and 2. These results are in reasonably good agreement with the reported values (refs. 7 to 9).

TABLE I.- SUMMARY OF CONSTITUENT LORENTZIAN PARAMETERS FOR PEAKS 1 AND 6 IN FeAl
MÖSSBAUER SPECTRA AT SEVERAL ALUMINUM CONCENTRATIONS

Aluminum concentration, atomic percent	Amplitudes of three Lorentzian peaks, peak counts			Positions of three Lorentzian peaks on x-axis, mm/sec		
	Absorption peak 1					
	A _{1,0}	A _{1,1}	A _{1,2}	P _{1,0}	P _{1,1}	P _{1,2}
0.5	4723 ± 63	189 ± 63	142 ± 63	-4.8167 ± 0.0024	-4.3644 ± 0.0604	-4.5570 ± 0.0864
1.0	4544 ± 66	364 ± 66	273 ± 66	-4.7960 ± 0.0026	-4.4115 ± 0.0338	-4.5870 ± 0.0476
1.5	4305 ± 66	517 ± 66	387 ± 66	-4.7902 ± 0.0029	-4.4209 ± 0.0249	-4.6812 ± 0.0358
2.0	4388 ± 66	702 ± 66	526 ± 66	-4.7942 ± 0.0029	-4.3967 ± 0.0194	-4.6035 ± 0.0267
	Absorption peak 6					
	A _{6,0}	A _{6,1}	A _{6,2}	P _{6,0}	P _{6,1}	P _{6,2}
0.5	5005 ± 55	200 ± 55	150 ± 55	+4.2396 ± 0.0016	+3.8770 ± 0.0429	+4.1251 ± 0.0621
1.0	4688 ± 48	375 ± 48	281 ± 48	+4.2337 ± 0.0020	+3.9353 ± 0.0213	+4.1702 ± 0.0369
1.5	4696 ± 48	564 ± 48	423 ± 48	+4.2349 ± 0.0017	+3.9001 ± 0.0147	+4.0607 ± 0.0204
2.0	4656 ± 45	745 ± 45	559 ± 45	+4.2314 ± 0.0017	+3.9058 ± 0.0109	+4.0412 ± 0.0149

TABLE II.- SUMMARY OF MEASURED VALUES OF ΔH FOR 1 nn AND 2 nn
ALUMINUM IMPURITY ATOMS IN FeAl ALLOYS

Aluminum concentration, atomic percent	ΔH , percent reduction, for -	
	1 nn shell	2 nn shell
0	0	0
.5	8.0 ± 1.3	3.9 ± 1.8
1.0	7.3 ± 0.8	2.9 ± 2.0
1.5	7.6 ± 0.6	2.9 ± 0.9
2.0	8.0 ± 0.4	4.3 ± 0.6
Average . . .	$a7.7 \pm 0.8$ percent	$a3.5 \pm 1.3$ percent

^aThese values should be compared with previously reported reductions of 8.0 and 4.0 percent, respectively (refs. 7 to 9).

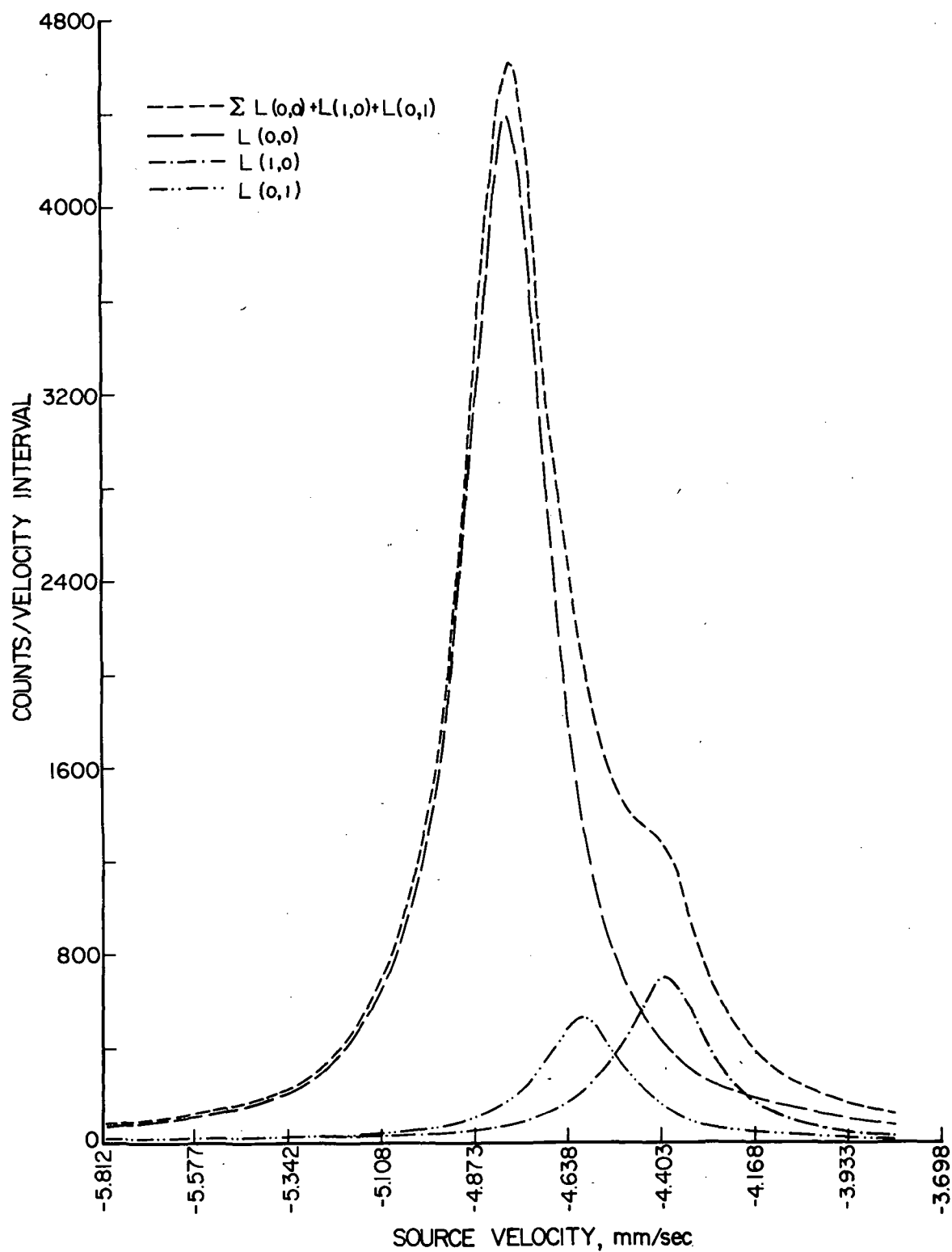


Figure 1.- Illustrative analysis of a composite Mössbauer hyperfine peak into three constituent peaks in FeAl alloy with 2.0 atomic percent aluminum.

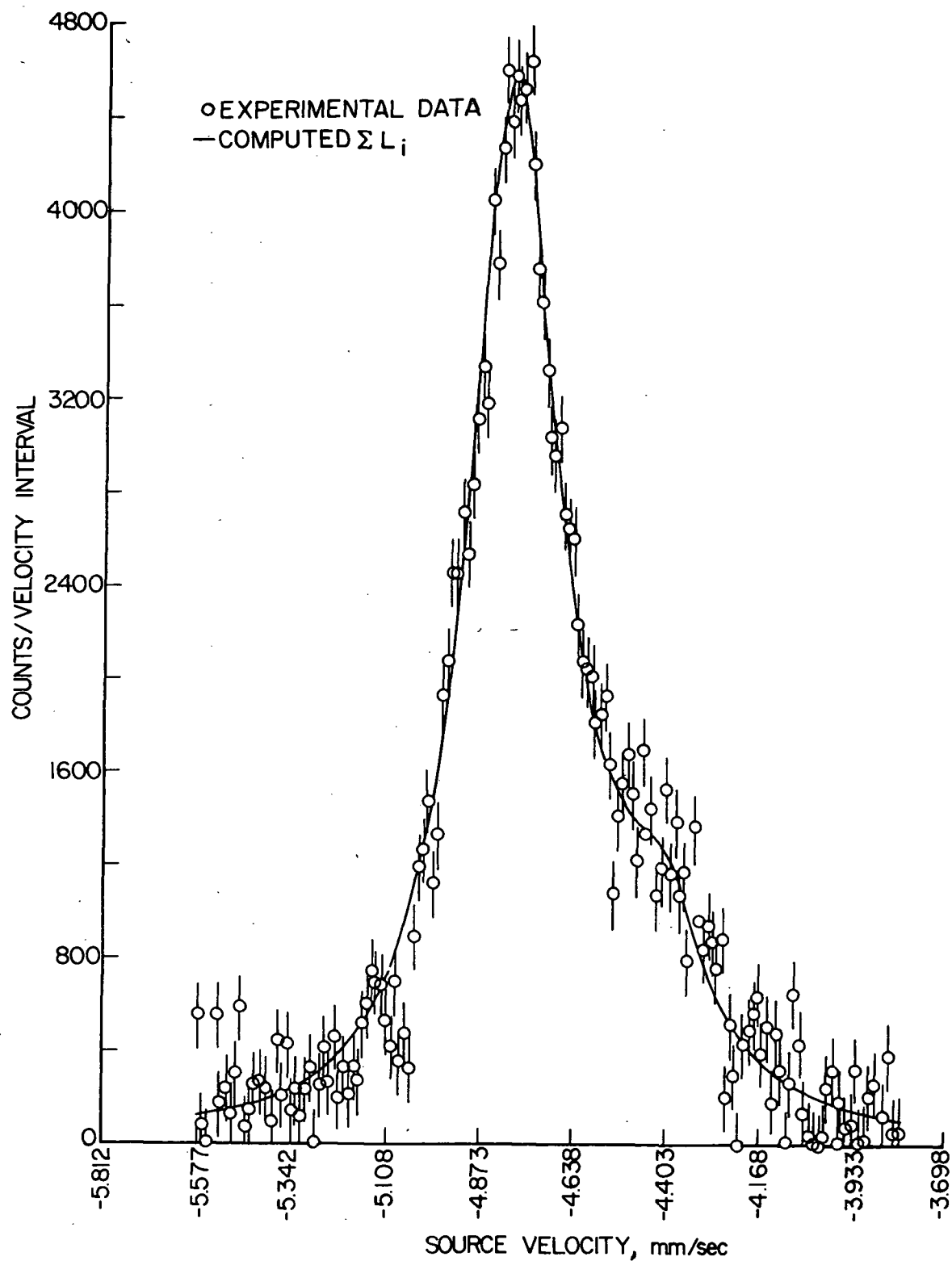


Figure 2.- Comparison between the computed and the experimentally observed spectra in FeAl alloy with 2.0 atomic percent aluminum.

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LEAST-SQUARES SOLUTION

The solution of equation (3) contains $3n$ parameters, which under theoretical conditions are constant. These parameters are $A_0, P_0, C_0, \dots, A_{n-1}, P_{n-1}, C_{n-1}$ where $C_0 = C_1 = \dots = C_{n-1} = \Gamma^2/4$.

Associated with L in equation (3) is some measurement error ϵ . Since this error exists, a computational method is needed which yields the best possible results with all the information available. The method of least squares, which is described subsequently, uses a minimum error criterion and has been used in the analysis of these Mössbauer data.

In general, equation (3) with the associated measurement errors can be written as

$$L_i = F(x_i, A_0, P_0, C_0, \dots, A_{n-1}, P_{n-1}, C_{n-1}) + \epsilon_i \quad (A1)$$

where F is a nonlinear function of the parameters, and in order to find an estimate to the parameters of the function, it must be linearized. Expanding equation (3) in a Taylor series about a nominal set of parameters and dropping the higher order terms result in the following linear approximation:

$$\begin{aligned} \Delta L_i &= L_i - L_{i,0} \\ &= b_{i,1}(A_0 - A_{0,0}) + b_{i,2}(P_0 - P_{0,0}) + b_{i,3}(C_0 - C_{0,0}) + \dots \\ &\quad + b_{i,3n-2}(A_{n-1} - A_{n-1,0}) + b_{i,3n-1}(P_{n-1} - P_{n-1,0}) \\ &\quad + b_{i,3n}(C_{n-1} - C_{n-1,0}) + \epsilon_i \end{aligned} \quad (A2)$$

where

$$\begin{aligned} b_{i,1} &= \left. \frac{\partial F_i}{\partial A_0} \right|_0 & b_{i,2} &= \left. \frac{\partial F_i}{\partial P_0} \right|_0 & b_{i,3} &= \left. \frac{\partial F_i}{\partial C_0} \right|_0 \\ &\vdots & & \vdots & & \vdots \\ b_{i,3n-2} &= \left. \frac{\partial F_i}{\partial A_{n-1}} \right|_0 & b_{i,3n-1} &= \left. \frac{\partial F_i}{\partial P_{n-1}} \right|_0 & b_{i,3n} &= \left. \frac{\partial F_i}{\partial C_{n-1}} \right|_0 \end{aligned}$$

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If α_j ($j = 1, 2, \dots, 3n$) represent the $3n$ parameters and

$$\Delta\alpha_1 = A_0 - A_{0,o} \quad \Delta\alpha_2 = P_0 - P_{0,o} \quad \Delta\alpha_3 = C_0 - C_{0,o}$$

$$\begin{array}{ccc} \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot \end{array}$$

$$\Delta\alpha_{3n-2} = A_{n-1} - A_{n-1,o} \quad \Delta\alpha_{3n-1} = P_{n-1} - P_{n-1,o} \quad \Delta\alpha_{3n} = C_{n-1} - C_{n-1,o}$$

equation (A2) can be put into the following form:

$$\Delta L_i = \sum_{j=1}^{3n} b_{i,j} \Delta\alpha_j + \epsilon_i \quad (A3)$$

For further considerations, the linear equation (A3) corresponding to the i th observation is expressed in matrix notation as

$$z_i = B_i \Delta\alpha + e_i \quad (A4)$$

where

$$z_i = \Delta y_i \quad B_i = [b_{i,1}, b_{i,2}, \dots, b_{i,3n}]$$

$$\Delta\alpha = \begin{bmatrix} \Delta\alpha_1 \\ \Delta\alpha_2 \\ \cdot \\ \cdot \\ \cdot \\ \Delta\alpha_{3n} \end{bmatrix} \quad e_i = [\epsilon_i]$$

Then for k ($k \geq 3n$) observations, there are k matrix equations of the form of equation (A4) which may be written

$$\bar{z} = \bar{B} \Delta\alpha + \bar{e} \quad (A5)$$

APPENDIX A

where

$$\bar{z} = \begin{bmatrix} z_1 \\ z_2 \\ \cdot \\ \cdot \\ \cdot \\ z_k \end{bmatrix} \quad \bar{B} = \begin{bmatrix} B_1 \\ B_2 \\ \cdot \\ \cdot \\ \cdot \\ B_k \end{bmatrix} \quad \bar{e} = \begin{bmatrix} e_1 \\ e_2 \\ \cdot \\ \cdot \\ \cdot \\ e_k \end{bmatrix}$$

The problem may be restated: Given \bar{z} and \bar{B} , find the best estimate $\hat{\Delta\alpha}$ for $\Delta\alpha$.

The best estimate $\hat{\Delta\alpha}$ is the value of $\Delta\alpha$ which minimizes the sum of the squares of the residuals $\bar{e}^T \bar{e}$ where

$$\bar{e}^T \bar{e} = (\bar{z} - \bar{B} \Delta\alpha)^T (\bar{z} - \bar{B} \Delta\alpha) \quad (A6)$$

In order to minimize equation (A6), the first variation δ with respect to $\Delta\alpha$ must vanish; that is,

$$\delta(\bar{e}^T \bar{e}) = \delta[(\bar{z} - \bar{B} \Delta\alpha)^T (\bar{z} - \bar{B} \Delta\alpha)] = -2(\bar{z}^T - \Delta\alpha^T \bar{B}^T) \bar{B} \delta(\Delta\alpha) = 0 \quad (A7)$$

Since $\delta(\Delta\alpha) \neq 0$, equation (A7) can be satisfied if

$$(\bar{z}^T - \Delta\alpha^T \bar{B}^T) \bar{B} = 0$$

or

$$\bar{B}^T \bar{B} \Delta\alpha = \bar{B}^T \bar{z} \quad (A8)$$

Solving for the estimate of $\Delta\alpha$ in equation (A8) gives

$$\hat{\Delta\alpha} = (\bar{B}^T \bar{B})^{-1} \bar{B}^T \bar{z} \quad (A9)$$

A second necessary condition for equation (A6) to be a minimum is that the second variation with respect to $\Delta\alpha$ be positive definite. Upon examination, the second variation is

$$\delta^2(\bar{e}^T \bar{e}) = 2 \delta(\Delta\alpha)^T \bar{B}^T \bar{B} \delta(\Delta\alpha)$$

which is positive definite. Therefore, equation (A9) is a valid expression for $\Delta\alpha$.

Since equation (A9) is based on a linear approximation with nominal $\alpha_{j,0}$, $\hat{\Delta\alpha}$ can be used to find the best estimates $\hat{\alpha}_j$. With the relationship $\alpha = \alpha_0 + \Delta\alpha$, the value of $\hat{\Delta\alpha}$ which minimized equation (A6) leads to a new nominal $\alpha_{j,0} = \alpha_{j,0} + \hat{\Delta\alpha}$. This process implies an iterative procedure which

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continues until $\hat{\Delta}\alpha \rightarrow 0$ and the value of $\alpha_{j,0}$ that leads to this result is the best estimate $\hat{\alpha}_j$ for α_j .

Error Analysis

Associated with the least-squares solution is the determination of the accuracy of the parameters α . When $\hat{\Delta}\alpha \rightarrow 0$ the best estimate $\hat{\alpha}^*$ of α is obtained. Associated with $\hat{\alpha}^*$ is the matrix $[\bar{B}^T \bar{B}]^{-1*}$. Multiplying $[\bar{B}^T \bar{B}]^{-1*}$ by the predicted variance σ^2 , where

$$\sigma^2 = \frac{\bar{e}^T \bar{e}}{(k - 3n)}$$

yields the covariance matrix V of the estimated parameters,

$$V = [\bar{B}^T \bar{B}]^{-1*} \sigma^2$$

By examining the diagonal elements of V , estimates of the error in α can be obtained. That is, the square roots of the diagonal elements of V are the estimates of the error bounds of α .

Partial Derivatives

For equation (A1),

$$F = \sum_{j=0}^{n-1} \frac{A_j C_j}{C_j + (P_j - x)^2}$$

The partial derivatives of F with respect to each parameter are as follows:

$$\left. \begin{aligned} \frac{\partial F}{\partial A_j} &= \frac{C_j}{C_j + (P_j - x)^2} \\ \frac{\partial F}{\partial P_j} &= \frac{-2A_j C_j (P_j - x)}{[C_j + (P_j - x)^2]^2} \\ \frac{\partial F}{\partial C_j} &= \frac{A_j (P_j - x)^2}{[C_j + (P_j - x)^2]^2} \end{aligned} \right\} \quad (j = 0, 1, \dots, n-1)$$

APPENDIX B

LANGLEY LIBRARY SUBROUTINE MATINV

Language: FORTRAN

Purpose: MATINV solves the matrix equation $AX = B$, where A is a square coefficient matrix and B is a matrix of constant vectors. The solution to a set of simultaneous equations, the matrix inverse, and the determinant may be obtained.

Use: CALL MATINV(MAX,N,A,M,B,IOP,DETERM,ISCALE,IPIVOT,IWK)

MAX	The maximum order of A as stated in the DIMENSION statement of the calling program
N	The order of A; $1 \leq N \leq \text{MAX}$
A	A two-dimensional array of coefficients. On return to the calling program, A^{-1} is stored in A.
M	The number of column vectors in B. On return to the calling program, X is stored in B if $M > 0$; for $M = 0$, the subroutine is used only for inversion.
B	A two-dimensional array of the constant vectors B. On return to the calling program, X is stored in B.
IOP	Option to compute the determinant: 0 Compute the determinant. 1 Do not compute the determinant.
DETERM	Gives the value of the determinant by the formula $\text{Det}(a) = 10^{(100 \times \text{ISCALE})(\text{DETERM})}$ when $\text{IOP} = 0$. For $\text{IOP} = 1$, the determinant is set to 1. For a singular matrix and $\text{IOP} = 0$ or $\text{IOP} = 1$, the determinant is set to zero.
ISCALE	A scale factor computed by the subroutine to keep the results of computation within the floating-point word size of the computer
IPIVOT	A one-dimensional array of temporary storage used by the subroutine
IWK	A two-dimensional array of temporary storage used by the subroutine

Restrictions: Arrays A, B, IPIVOT, and INDEX have variable dimensions in the subroutine. The maximum size of these arrays must be specified in a DIMENSION statement of the calling program as A(MAX,MAX), B(MAX,M), IPIVOT(MAX), and IWK(MAX,2). The original matrices A and B are destroyed. They must be saved

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by the user if there is further need for them. The determinant is set to zero for a singular matrix.

Method: Jordan's method is used to reduce a matrix A to the identity matrix I through a succession of elementary transformations $\ell_n, \ell_{n-1}, \dots, \ell_1$. If these transformations are simultaneously applied to I and to a matrix B of constant vectors, the results are A^{-1} and X where $AX = B$. Each transformation is selected so that the largest element is used in the pivotal position. (See ref. (a).)

Accuracy: Total pivotal strategy is used to minimize the rounding errors; however, the accuracy of the final results depends upon how well-conditioned the original matrix is. A return with $DETERM \neq 0$ does not guarantee accuracy in the solutions of inverse.

Reference: (a) Fox, L.: An Introduction to Numerical Linear Algebra. Oxford Univ. Press, 1965.

Storage: 516 octal locations

Subroutine date: January 1, 1975

APPENDIX C

SAMPLE CASE

The printout from a sample case is presented in this appendix. The case is an FeAl alloy with 2 percent aluminum.

Listing of input:

```
IT =25  M= 171  N= 4  EPS= .1000000000E-01
DELETION FLAGS... 0=DELETE, 1=SOLVE
      1      1      0
      0      1      0
      0      1      0
      0      1      0
```

```
P( 1) --.3900000000E+04
P( 2) --.4800000000E+01
P( 3) --.1634925300E-01
P( 4) --.6240000000E+03
P( 5) --.4420000000E+01
P( 6) --.1634925300E-01
P( 7) --.4680000000E+03
P( 8) --.4690000000E+01
P( 9) --.1634925300E-01
P(10) --.4110892650E+04
P(11) --.2791025610E+01
P(12) --.1683621600E-01
PARABOLA PARAMETERS PA=
```

```
.41848235E+02  P8= .32715052E+01  PC= .43602308E+05
```

X

```
--.58003914E+01
--.57299413E+01
--.56594912E+01
--.55890411E+01
--.55185910E+01
--.54481409E+01
--.53776908E+01
--.53072407E+01
--.52367906E+01
--.51663405E+01
--.50958904E+01
--.50254403E+01
--.49549902E+01
--.48845401E+01
--.48140900E+01
--.47436399E+01
--.46731898E+01
--.46027397E+01
--.45322896E+01
--.44618395E+01
--.43913894E+01
--.43209393E+01
--.42504892E+01
--.41800391E+01

--.57886497E+01
--.57181996E+01
--.56477495E+01
--.55772994E+01
--.55068493E+01
--.54363992E+01
--.53659491E+01
--.52954990E+01
--.52250489E+01
--.51545988E+01
--.50841487E+01
--.50136986E+01
--.49432485E+01
--.48727984E+01
--.48023483E+01
--.47318982E+01
--.46614481E+01
--.45909980E+01
--.45205480E+01
--.44500979E+01
--.43796478E+01
--.43091977E+01
--.42387476E+01
--.41682975E+01

--.57769080E+01
--.57064579E+01
--.56360078E+01
--.55655577E+01
--.54951076E+01
--.54246575E+01
--.53542074E+01
--.52837573E+01
--.52133072E+01
--.51428571E+01
--.50724071E+01
--.50019570E+01
--.49315069E+01
--.48610568E+01
--.47906067E+01
--.47201566E+01
--.46497065E+01
--.45792564E+01
--.45088063E+01
--.44383562E+01
--.43679061E+01
--.42974560E+01
--.42270059E+01
--.41565558E+01

--.57651663E+01
--.56947162E+01
--.56242661E+01
--.55538161E+01
--.54833660E+01
--.54129159E+01
--.53424658E+01
--.52720157E+01
--.52015656E+01
--.51311155E+01
--.50606654E+01
--.49902153E+01
--.49197652E+01
--.48493151E+01
--.47788650E+01
--.47084149E+01
--.46379648E+01
--.45675147E+01
--.44970646E+01
--.44266145E+01
--.43561644E+01
--.42857143E+01
--.42152642E+01
--.41448141E+01

--.57534247E+01
--.56829746E+01
--.56125245E+01
--.55420744E+01
--.54716243E+01
--.54011742E+01
--.53307241E+01
--.52602740E+01
--.51898239E+01
--.51193738E+01
--.50489237E+01
--.49784736E+01
--.49080235E+01
--.48375734E+01
--.47671233E+01
--.46966732E+01
--.46262231E+01
--.45557730E+01
--.44853229E+01
--.44148728E+01
--.43444227E+01
--.42739726E+01
--.42035225E+01
--.41330724E+01

--.57416830E+01
--.56712329E+01
--.56007828E+01
--.55303327E+01
--.54598826E+01
--.53894325E+01
--.53189824E+01
--.52485323E+01
--.51780822E+01
--.51076321E+01
--.50371820E+01
--.49667319E+01
--.48962818E+01
--.48258317E+01
--.47553816E+01
--.46849315E+01
--.46144814E+01
--.45440313E+01
--.44735812E+01
--.44031311E+01
--.43326810E+01
--.42622309E+01
--.41917808E+01
--.41213307E+01
```

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--.41095890E+01	--.40978474E+01	--.40861057E+01	--.40743640E+01	--.40626223E+01	--.40508806E+01
--.40391389E+01	--.40273973E+01	--.40156556E+01	--.40039139E+01	--.39921722E+01	--.39804305E+01
--.39686889E+01	--.39569472E+01	--.39452059E+01	--.39334938E+01	--.39217221E+01	--.39099804E+01
--.38982388E+01	--.38864971E+01	--.38747558E+01	--.38630137E+01	--.38512720E+01	--.38393930E+01
--.38277887E+01	--.38160470E+01	--.38043053E+01			
.44336000E+05	.44795000E+05	.44356400E+05	.44320900E+05	.44364000E+05	.44916000E+05
.44992000E+05	.44808000E+05	.44026000E+05	.44841000E+05	.44698000E+05	.44997000E+05
.44940000E+05	.44925000E+05	.44089000E+05	.44814000E+05	.44952000E+05	.44807000E+05
.44629000E+05	.44319000E+05	.44791000E+05	.45046000E+05	.44726000E+05	.44292000E+05
.44690000E+05	.44602000E+05	.44707000E+05	.44529000E+05	.44138000E+05	.44752000E+05
.44602000E+05	.44597000E+05	.44951000E+05	.44559000E+05	.44578000E+05	.44702000E+05
.44334000E+05	.44564000E+05	.44344000E+05	.44628000E+05	.44533000E+05	.44636000E+05
.44510000E+05	.44417000E+05	.44842000E+05	.44488000E+05	.44323000E+05	.44466000E+05
.44255000E+05	.44527000E+05	.44376000E+05	.44502000E+05	.44367000E+05	.44428000E+05
.44173000E+05	.44084000E+05	.44393500E+05	.44397900E+05	.44398200E+05	.44139000E+05
.44242000E+05	.44395700E+05	.44296000E+05	.44416800E+05	.44311000E+05	.44374200E+05
.44346000E+05	.44335500E+05	.44313900E+05	.44393300E+05	.44327000E+05	.44267400E+05
.42588000E+05	.42136000E+05	.44213800E+05	.41874000E+05	.42042000E+05	.41742000E+05
.41448000E+05	.41218000E+05	.41378000E+05	.40498000E+05	.40761000E+05	.40267000E+05
.39944000E+05	.40152000E+05	.39950000E+05	.40054000E+05	.39992000E+05	.39870000E+05
.40309000E+05	.40744000E+05	.40892000E+05	.41169000E+05	.41453000E+05	.41523000E+05
.41396000E+05	.41769000E+05	.41821000E+05	.41857000E+05	.42219000E+05	.42374000E+05
.42411000E+05	.42437000E+05	.42635000E+05	.42591000E+05	.42501000E+05	.42796000E+05
.43340000E+05	.42994000E+05	.42862000E+05	.42733000E+05	.42904000E+05	.43183000E+05
.42696000E+05	.43059000E+05	.42943000E+05	.43320000E+05	.43201000E+05	.42846000E+05
.43207000E+05	.42970000E+05	.43291000E+05	.43188000E+05	.43564000E+05	.42972000E+05
.43368000E+05	.43508000E+05	.43390000E+05	.43456000E+05	.43573000E+05	.43437000E+05
.44118000E+05	.43795000E+05	.44013000E+05	.44319000E+05	.4410000E+05	.43789000E+05
.43729000E+05	.43650000E+05	.43889000E+05	.43766000E+05	.43995000E+05	.43802000E+05
.43934000E+05	.44248000E+05	.43987000E+05	.43588000E+05	.43955000E+05	.43789000E+05
.44191000E+05	.44324000E+05	.44213000E+05	.44182000E+05	.43967000E+05	.44109000E+05
.44361000E+05	.44024000E+05	.44110000E+05	.44099000E+05	.43847000E+05	.43864000E+05
.44248000E+05	.43948000E+05	.43897000E+05	.43927000E+05		.44245000E+05
.44088000E+05	.44080000E+05	.44198000E+05		.44026000E+05	.43749000E+05

Y

Listing of output:

ITERATION 1			
SUM-OF-SQUARES	.1835345E+08		
VARIANCES	.8345458E-01	.1384727E-09	.6028772E-08
CORRELATIONS			.1344064E-07
.1000000E+01	.1007749E+00	-.3479139E+00	-.5170101E+00
.1007749E+00	.1000000E+01	.6904106E-01	-.2328584E+00
-.3479139E+00	.6904106E-01	.1000000E+01	.3510218E+00
-.5170101E+00	-.2328584E+00	.3510218E+00	.1000000E+01
ELEMENT NAME	OLD VALUE	INCREMENT	NEW VALUE
A0	-.390000000000000E+04	-.57820267848886E+03	-.44782026784889E+04
P0	-.480000000000000E+01	.44869803235125E-02	-.47955130196765E+01
C0	.16349253000000E-01	0.	.16349253000000E-01
A1	-.62400000000000E+03	0.	-.62400000000000E+03
P1	-.44200000000000E+01	.29948746082674E-01	-.43900512539173E+01
C1	.16349253000000E-01	0.	.16349253000000E-01
A2	-.46800000000000E+03	0.	-.46800000000000E+03
P2	-.46900000000000E+01	.11835242341913E+00	-.45716475765809E+01
C2	.16349253000000E-01	0.	.16349253000000E-01
ITERATION 2			
SUM-OF-SQUARES	.1378942E+08		
VARIANCES	.7690413E-01	.1078611E-09	.5718133E-08
CORRELATIONS			.1219603E-07
.1000000E+01	-.1658604E+00	-.2943244E+00	-.4609360E+00
-.1658604E+00	.1000000E+01	.2318155E+00	.3080394E+00
.2943244E+00	.2318155E+00	.1000000E+01	.3003302E+00
-.4609360E+00	.3080394E+00	.3003302E+00	.1000000E+01
ELEMENT NAME	OLD VALUE	INCREMENT	NEW VALUE
A0	-.44782026784889E+04	-.28104231532339E+01	-.44810131016421E+04
P0	-.47955130196765E+01	.36437000976543E-02	-.47918693195788E+01
C0	.16349253000000E-01	0.	.16349253000000E-01
A1	-.62400000000000E+03	0.	-.62400000000000E+03
P1	-.43900512539173E+01	-.27985378597092E-02	-.43928497917770E+01
C1	.16349253000000E-01	0.	.16349253000000E-01
A2	-.46800000000000E+03	0.	-.46800000000000E+03
P2	-.45716475765809E+01	.48792464116875E-03	-.45711596519397E+01
C2	.16349253000000E-01	0.	.16349253000000E-01

ITERATION 3

SUM-OF-SQUARES .1363877E+08
 VARIANCES .7730562E-01 .1076307E-09 .5710496E-08 .1216130E-07
 CORRELATIONS
 .100000E+01 -.1664750E+00 -.2964624E+00 -.4634974E+00
 -.1664750E+00 .100000E+01 .2334817E+00 .3043375E+00
 -.2964624E+00 .2334817E+00 .100000E+01 .2925864E+00
 -.4634974E+00 .3043375E+00 .2925864E+00 .100000E+01

ELEMENT NAME	OLD VALUE	INCREMENT	NEW VALUE
A0	-.44810131016421E+04	-.25912261987865E+01	-.44836043278408E+04
P0	-.47918693195788E+01	.20025174772088E-03	-.47916690678311E+01
C0	.16349253000000E-01	0.	.16349253000000E-01
A1	-.62400000000000E+03	0.	-.62400000000000E+03
P1	-.4392849791770E+01	.93891964939949E-03	-.43919108721276E+01
C1	.16349253000000E-01	0.	.16349253000000E-01
A2	-.46800000000000E+03	0.	-.46800000000000E+03
P2	-.45711596519397E+01	.10069953363541E-02	-.45701526566033E+01
C2	.16349253000000E-01	0.	.16349253000000E-01

ITERATION 4

SUM-OF-SQUARES .1363831E+08
 VARIANCES .7717123E-01 .1075208E-09 .5704656E-08 .1214764E-07
 CORRELATIONS
 .100000E+01 -.1661490E+00 -.2952762E+00 -.4622401E+00
 -.1661490E+00 .100000E+01 .2328269E+00 .3048209E+00
 -.2952762E+00 .2328269E+00 .100000E+01 .2916618E+00
 -.4622401E+00 .3048209E+00 .2916618E+00 .100000E+01

ELEMENT NAME	OLD VALUE	INCREMENT	NEW VALUE
A0	-.44836043278408E+04	.38579619152337E-01	-.44835657482217E+04
P0	-.47916690678311E+01	.67290512481311E-05	-.47916623387798E+01
C0	.16349253000000E-01	0.	.16349253000000E-01
A1	-.62400000000000E+03	0.	-.62400000000000E+03
P1	-.43919108721276E+01	-.13291509969003E-03	-.43920437872273E+01
C1	.16349253000000E-01	0.	.16349253000000E-01
A2	-.46800000000000E+03	0.	-.46800000000000E+03
P2	-.45701526566033E+01	.45632667666979E-04	-.45701070239356E+01
C2	.16349253000000E-01	0.	.16349253000000E-01

APPENDIX C

ITERATION 5

SUM-OF-SQUARES .1363831E+08
 VARIANCES .7715814E-01 .1075207E-09 .5702837E-08 .1214245E-07
 CORRELATIONS
 .1000000E+01 -.1660926E+00 -.2950863E+00 -.4620542E+00
 -.1660926E+00 .1000000E+01 .2327451E+00 .3047399E+00
 -.2950863E+00 .2327451E+00 .1000000E+01 .2910326E+00
 -.4620542E+00 .3047399E+00 .2910326E+00 .1000000E+01

ELEMENT NAME	OLD VALUE	INCREMENT	NEW VALUE
A0	-.44835657482217E+04	-.31607363410762E-01	-.44835973555851E+04
P0	-.47916623387798E+01	.11911228341849E-05	-.47916611476370E+01
C0	.16349253000000E-01	0.	.16349253000000E-01
A1	-.62400000000000E+03	0.	-.62400000000000E+03
P1	-.43920437872273E+01	.24817587566795E-04	-.43920189696397E+01
C1	.16349253000000E-01	0.	.16349253000000E-01
A2	-.46800000000000E+03	0.	-.46800000000000E+03
P2	-.45701070239356E+01	.15072347489422E-04	-.45700919515881E+01
C2	.16349253000000E-01	0.	.16349253000000E-01

ITERATION 6

SUM-OF-SQUARES .1363831E+08
 VARIANCES .7715624E-01 .1075195E-09 .5702833E-08 .1214250E-07
 CORRELATIONS
 .1000000E+01 -.1660893E+00 -.2950742E+00 -.4620403E+00
 -.1660893E+00 .1000000E+01 .2327368E+00 .3047344E+00
 -.2950742E+00 .2327368E+00 .1000000E+01 .2910531E+00
 -.4620403E+00 .3047344E+00 .2910531E+00 .1000000E+01

ELEMENT NAME	OLD VALUE	INCREMENT	NEW VALUE
A0	-.44835973555851E+04	.29495073000536E-02	-.44835944060778E+04
P0	-.47916611476570E+01	-.44142840199190E-07	-.47916611917998E+01
C0	.16349253000000E-01	0.	.16349253000000E-01
A1	-.62400000000000E+03	0.	-.62400000000000E+03
P1	-.43920189696397E+01	-.40147329391525E-05	-.43920229843726E+01
C1	.16349253000000E-01	0.	.16349253000000E-01
A2	-.46800000000000E+03	0.	-.46800000000000E+03
P2	-.45700919515881E+01	-.3448907996556E-06	-.45700922964789E+01
C2	.16349253000000E-01	0.	.16349253000000E-01

ALL CORRECTIONS LESS THAN .1000000E-01 STOP.

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16. Abstract A computer program has been developed for analyzing unresolved Mössbauer hyperfine spectra resulting from the existence of several local environments in dilute binary iron alloys. This program is an extension of an earlier program which had not been adapted for analyzing such unresolved compound spectra. The program is written in FORTRAN IV language for the Control Data CYBER 170 series digital computer system with network operating system (NOS) 1.1. With the present dimensions, the program requires approximately 36000 octal locations of core storage. A typical case involving two innermost coordination shells in which the amplitudes and the peak positions of all three components are estimated in 25 iterations requires 30 seconds on CYBER 173. The program has been applied to determine the effects of various near-neighbor impurity shells on hyperfine fields in dilute FeAl alloys.					
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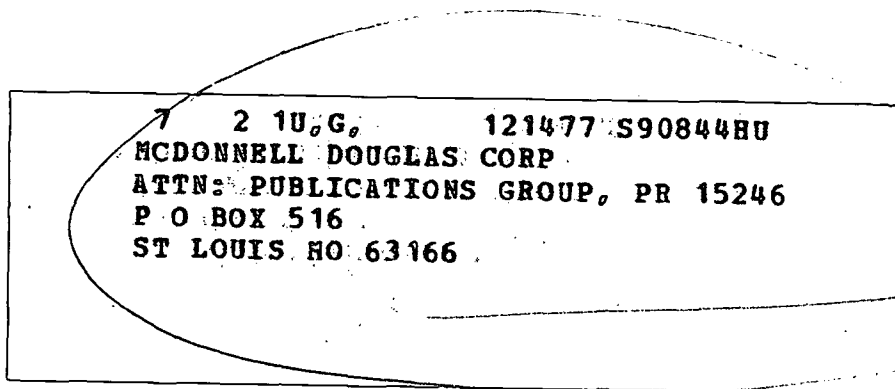
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